Energetics of fluctuations in non-equilibrium Langevin systems

Dept. of Physics, Kyoto Univ. Takahiro Harada [1]

平衡状態にある系の揺らぎの大きさは、摂動に対する応答関数に系の温度を掛けたものに等しいことはよく知られている（揺動散逸関係）。一方、外界からエネルギー入力を受けて、非平衡定常状態に維持されている系については、等温系であっても揺動散逸関係が成り立たない事が知られており、その破れの物理的意義が議論されている。本講演では、ダイナミクスがLangevin方程式で記述されるような非平衡系について、揺動散逸関係の破れの度合いと、系が環境へと散逸するエネルギーの量とを結びつける等式関係があることを示す。

For systems in equilibrium, it has been established as the *fluctuation-dissipation theorem* that the magnitude of fluctuations is equal to the the response function against a small perturbation multiplied by the temperature of the system. On the other hand, for systems maintained at a non-equilibrium steady state by external driving forces, it has been realized that the similar relation does not hold in general even in an isothermal case. In the present paper, we show that there is an equality betweeen an extent of violation of the fluctuation-dissipation relation (FDR) and the rate of energy dissipation into the environment for non-equilibrium systems that can be described by Langevin equations [1].

As a simple example, we consider a system where N spherical colloidal particles in a three dimensional aqueous solution are driven by an constant external force $f\boldsymbol{e}_x$ [2]. Let us denote the coordinates of the particles by $\Gamma = \{x_i\}$ $(i = 0, \cdots, 3N-1)$, where $\boldsymbol{r}_\mu \equiv (x_{3\mu}, x_{3\mu+1}, x_{3\mu+2})$ represents the position of the μ-th particle $(\mu = 0, \cdots, N-1)$. Then, a widely used model describing the motion of the particles is provided as [3]

$$\gamma \dot{x}_i(t) = F_i(\Gamma(t)) + \xi_i(t) + \varepsilon f_i^{\mathrm{p}}(t), \tag{1}$$

where γ is the friction coefficient of a particle and

$$F_i(\Gamma) \equiv \sum_{\mu=0}^{N-1} f\delta_{i,3\mu} - \partial_{x_i} \sum_{\mu=0}^{N-1} U(\boldsymbol{r}_\mu) - \partial_{x_i} \sum_{\mu=0}^{N-1}\sum_{\nu=0}^{N-1} \frac{V_{\mu\nu}(|\boldsymbol{r}_\mu - \boldsymbol{r}_\nu|)}{2} \tag{2}$$

represents the driving force, a single-body conservative force and two-body interactions. The noise, $\xi_i(t)$, satisfies that $\langle \xi_i(t)\xi_j(s)\rangle = 2\gamma T\delta_{ij}\delta(t-s)$. The last term in the r.h.s. of (1) with

[1] E-mail: t.harada@scphys.kyoto-u.ac.jp

$\varepsilon \ll 1$ denotes a perturbation force to investigate the response of the system [see (6)]. For this model, it is found that the energy dissipated into the solvent, $J(t)$, is expressed as

$$J(t)\mathrm{d}t \equiv \sum_{i=0}^{3N-1} [\gamma \dot{x}_i(t) - \xi_i(t)] \circ \mathrm{d}x_i(t), \tag{3}$$

where $\circ$ denotes the multiplication in the Stratonovich sense [4].

In the present paper, we show that the following identity holds:

$$\langle J \rangle_0 = \sum_{i=0}^{3N-1} \gamma \left\{ \langle \dot{x}_i \rangle_0^2 + \int_{-\infty}^{\infty} \left[\tilde{C}_{ii}(\omega) - 2T\tilde{R}'_{ii}(\omega) \right] \frac{\mathrm{d}\omega}{2\pi} \right\}, \tag{4}$$

where $\langle \cdots \rangle_\varepsilon$ denotes the ensemble average with the parameter ε fixed. $C_{ij}(t)$ are the velocity correlation functions defined as

$$C_{ij}(t) \equiv \langle [\dot{x}_i(t) - \langle \dot{x}_i \rangle_0][\dot{x}_j(0) - \langle \dot{x}_j \rangle_0] \rangle_0 , \tag{5}$$

and $R_{ij}(t)$ are the response functions defined as

$$\langle \dot{x}_i(t) \rangle_\varepsilon = \langle \dot{x}_i \rangle_0 + \varepsilon \sum_{j=0}^{3N-1} \int_{-\infty}^{t} R_{ij}(t-s) f_j^{\mathrm{p}}(s) \mathrm{d}s + O(\varepsilon^2). \tag{6}$$

It is found that the r.h.s. of (4) represents an extent of the FDR violation and thus it vanishes in equilibrium. Therefore, (4) expresses the equivalence between the rate of energy dissipation into the environment and the extent of the FDR violation. It should be also noted that this result is rigorous and is valid independ of the magnitude of the driving force. Since this equality is closed with experimentally measurable quantities, it serves as a "check sum" to quantitatively test the relevance of the Langevin-type model (1) to describe non-equilibrium phenomena.

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